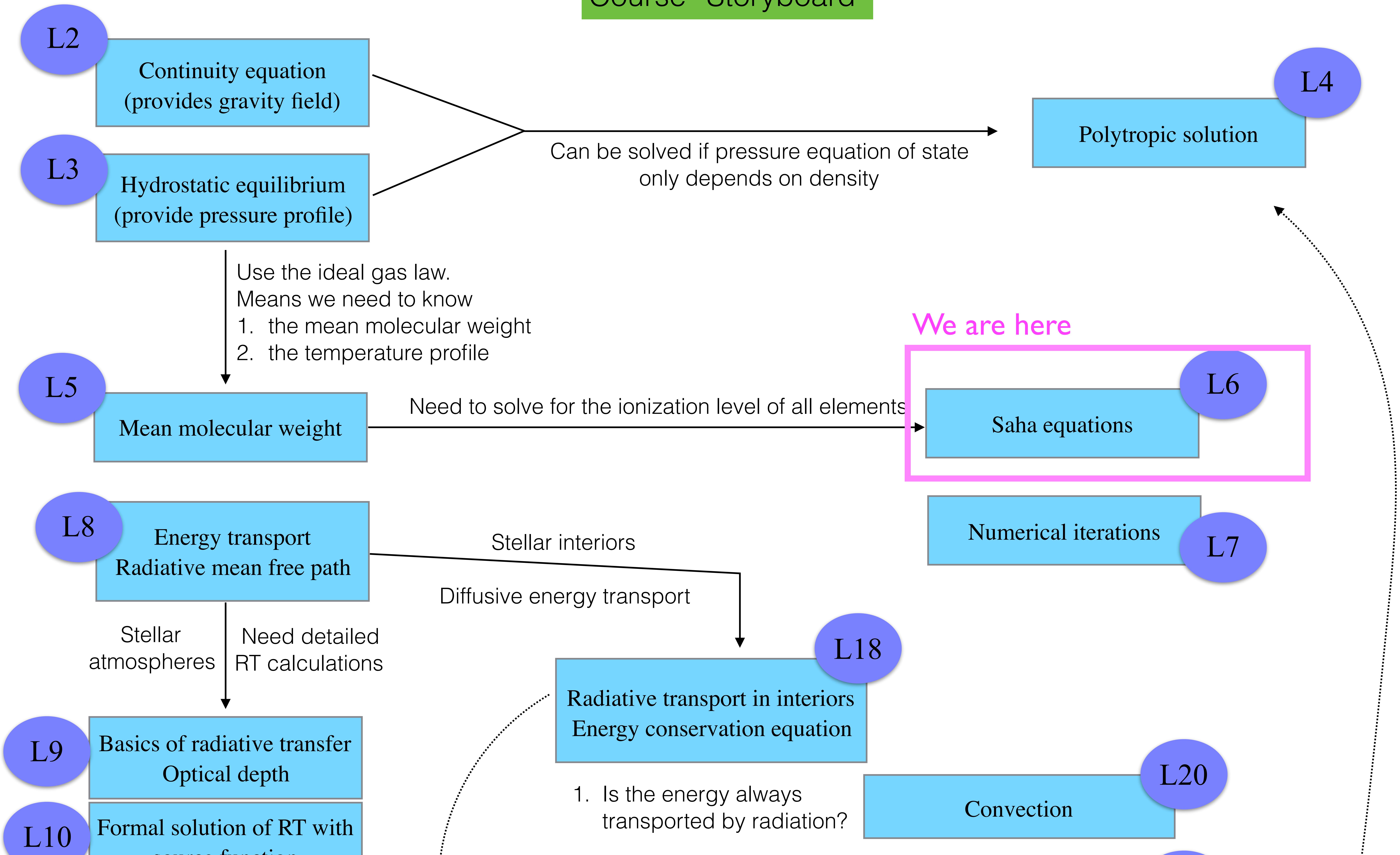
Week 3 Thursday

L-6

Saha

Course “Storyboard”



Continuity equation

$$\frac{dM_r(r)}{dr} = 4\pi r^2 \rho(r)$$

$M_r(r)$ $P(r)$ $T(r)$

$\rho(r)$ $\mu(r)$

We assume:
Initial comp: X_i

Hydrostatic equilibrium

$$\frac{dP(r)}{dr} = -\rho(r)\frac{GM_r(r)}{r^2}$$

Ideal gas law

$$P(r) = \frac{\rho(r)}{\mu(r) m_H} kT(r)$$

Mean molecular weight

$$\mu(r) = f(\mathrm{comp}, T(r), P(r))$$

$$\frac{1}{\mu} = \frac{1}{\mu_{\mathrm{ion}}} + \frac{1}{\mu_{\mathrm{e}}}$$

$$\frac{1}{\mu_{\mathrm{ion}}} = \sum_i \frac{X_i}{A_i} \qquad \frac{1}{\mu_{\mathrm{e}}} = \sum_i \frac{X_i}{A_i} Z_i y_i$$

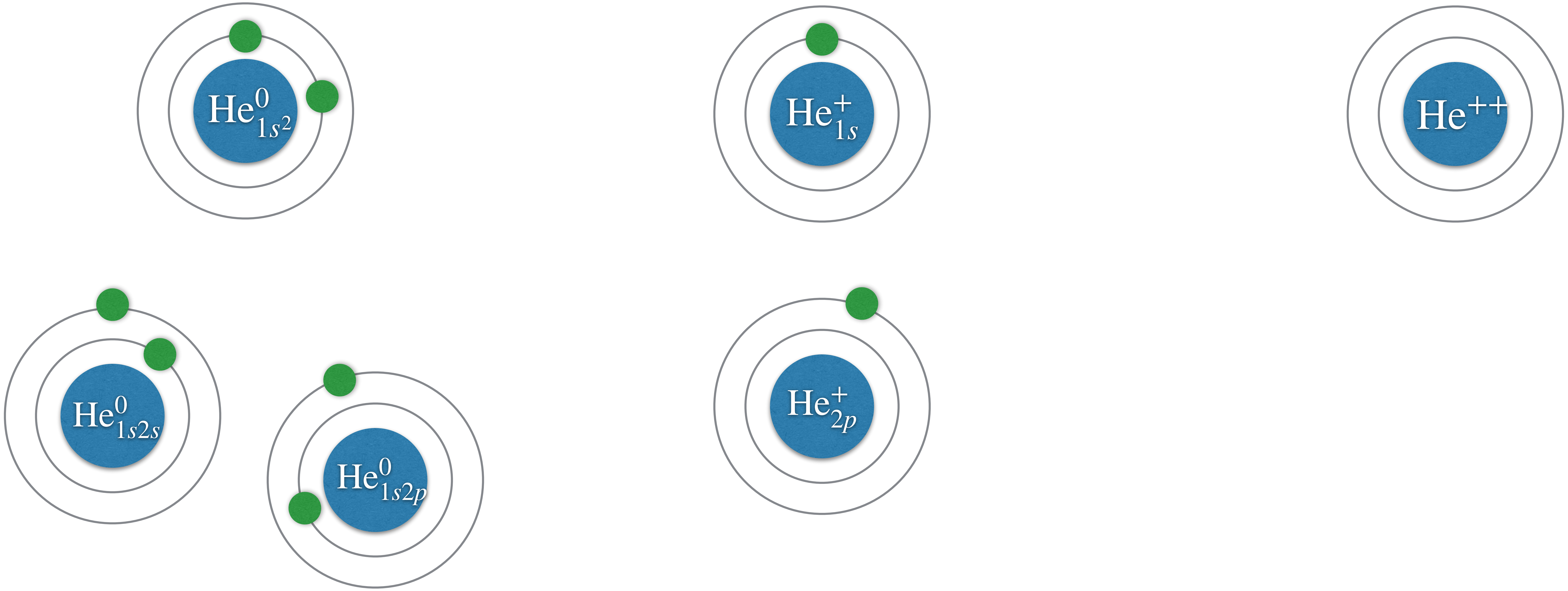
element

Ionization state

$$A^{r}_{s_a}$$

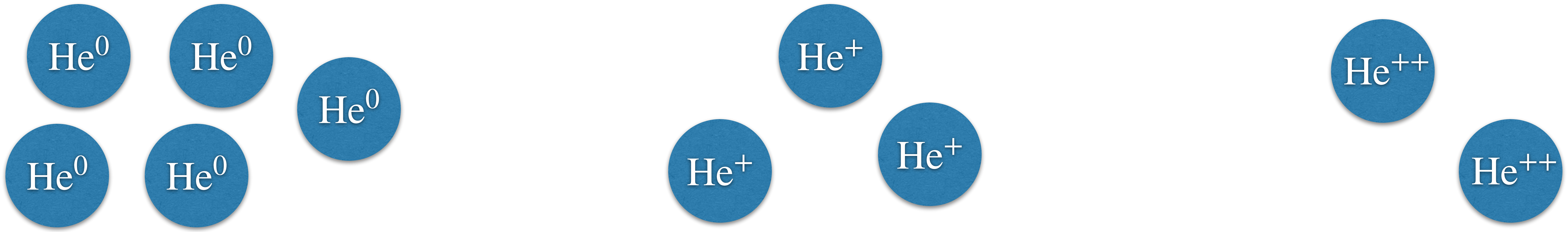
Excitation state

(Energy level of the still bound electrons)



How many free electrons are there?

0 3 4



$$n_e = 0\ n_{He^0} + 1\ n_{He^+} + 2\ n_{He^{++}}$$

What if they were all ionized?

$$n_{e \text{ all ionized}} = 10 \quad = 2\ n_{He} = Z_{He}\ n_{He}$$

So:

$$y_i = \frac{\#\text{ of free electrons/volume}}{\#\text{ of free electron if all ionized/volume}} = \frac{1}{Z_i}\left[\ 1\ \frac{n_{He^+}}{n_{He}} + \ 2\ \frac{n_{He^{++}}}{n_{He}}\right]$$

We need to use the ideal gas law $\rightarrow$ We need to calculate μ $\rightarrow$ We need to know y_i

$$P(r) = \frac{\boxed{\rho(r)}}{\boxed{\mu(r)} m_H} kT(r)$$

$$\boxed{\mu(r)} = f(\mathrm{comp}, T(r), P(r))$$

$$\frac{1}{\mu_e} = \sum_i \frac{X_i}{A_i} Z_i \, y_i$$

$\downarrow$

We need to know all of the $\frac{n_A^r}{n_A}$

Goal: find $\frac{n_A^r}{n_A}$ $\longleftarrow$ $\frac{n_{\mathrm{H}}^o}{n_{\mathrm{H}}}$ $\frac{n_{\mathrm{H}}^+}{n_{\mathrm{H}}}$ $\frac{n_{\mathrm{He}}^o}{n_{\mathrm{He}}}$ $\frac{n_{\mathrm{He}}^+}{n_{\mathrm{He}}}$ $\frac{n_{\mathrm{He}}^{++}}{n_{\mathrm{He}}}$ $\ldots$

x_{H}^o x_{H}^+ x_{He}^o x_{He}^+ x_{He}^{++} $\ldots$

element

Ionization stage

$$A^{r}_{s_a}$$

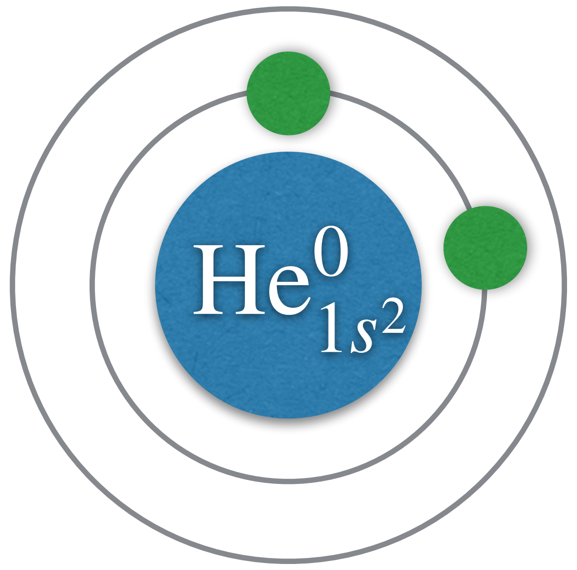
Excitation stage

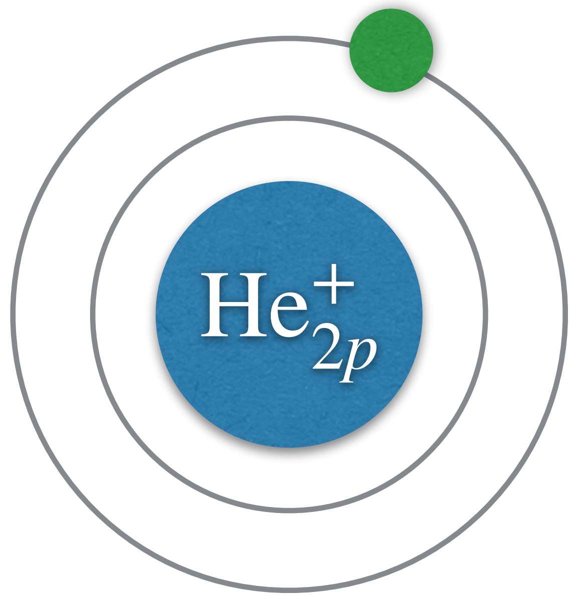
(Energy level of the still bound electrons)

A single ionization 'reaction'

A certain amount of

$$A^{r}_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^{-}$$

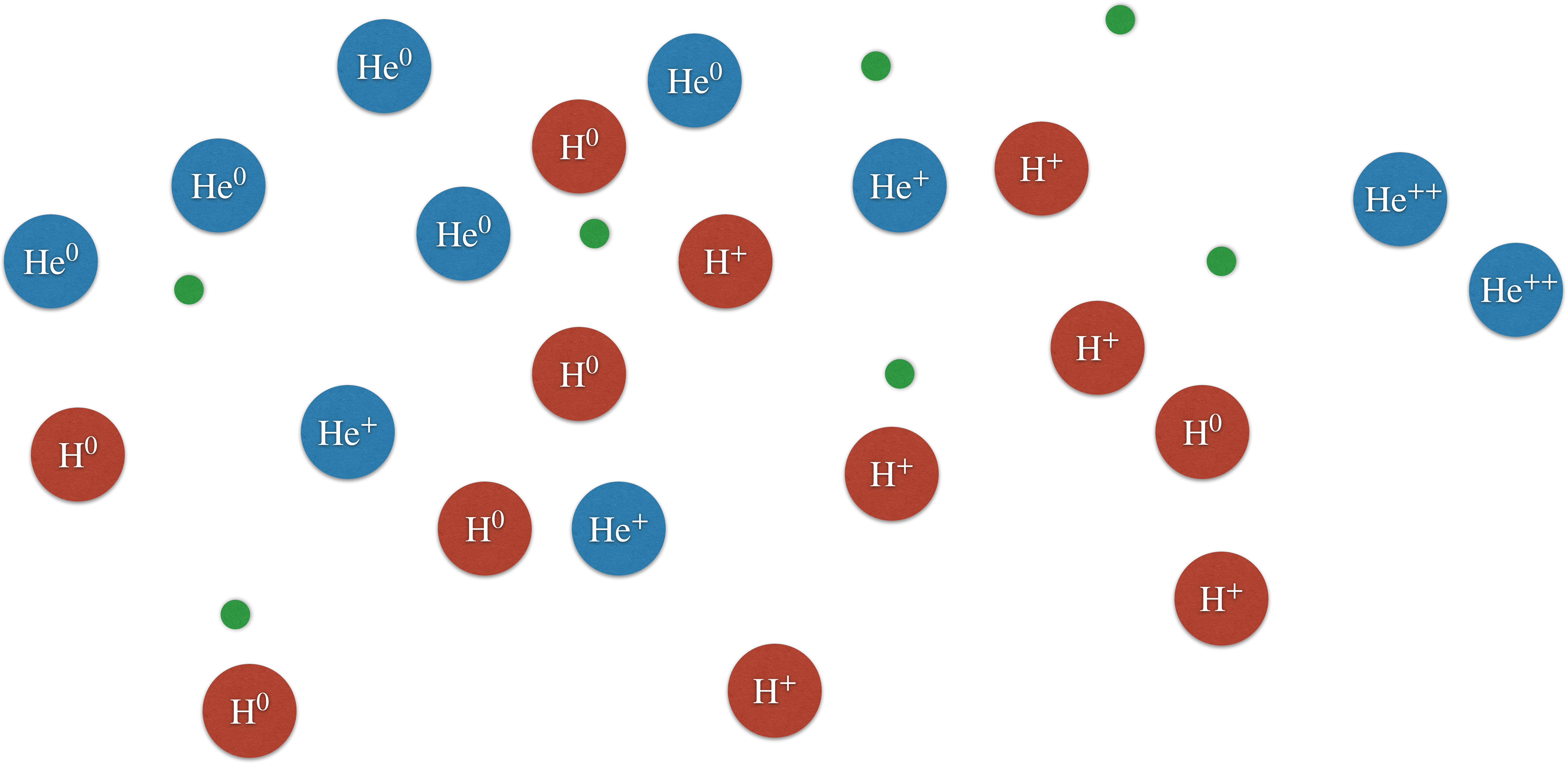




Remaining electrons are not necessarily in the original configuration…

Statistical mechanics:

If we have a large amount of particles, and the energy exchanges are mostly caused by collisions, then the number of particles in each ionization/excitation state can be related to temperature



$$A^{r}_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^{-}$$

$$\mathrm{H}^{o}_{1s} + \text{energy} \Longleftrightarrow \mathrm{H}^{+} + e^{-}$$

$$\mathrm{H}^{o}_{2s} + \text{energy} \Longleftrightarrow \mathrm{H}^{+} + e^{-}$$

$$\mathrm{He}^{o}_{1s^2} + \text{energy} \Longleftrightarrow \mathrm{He}^{+}_{1s} + e^{-}$$

$$\mathrm{He}^{o}_{1s2s} + \text{energy} \Longleftrightarrow \mathrm{He}^{+}_{1s} + e^{-}$$

$$\mathrm{He}^{o}_{1s2p} + \text{energy} \Longleftrightarrow \mathrm{He}^{+}_{2p} + e^{-}$$

$$\ldots$$

Same "pool" of free electrons

This is a problem where all of the equations are coupled.

$$A^r_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^-$$

Goal: find $\dfrac{n^r_A}{n_A}$

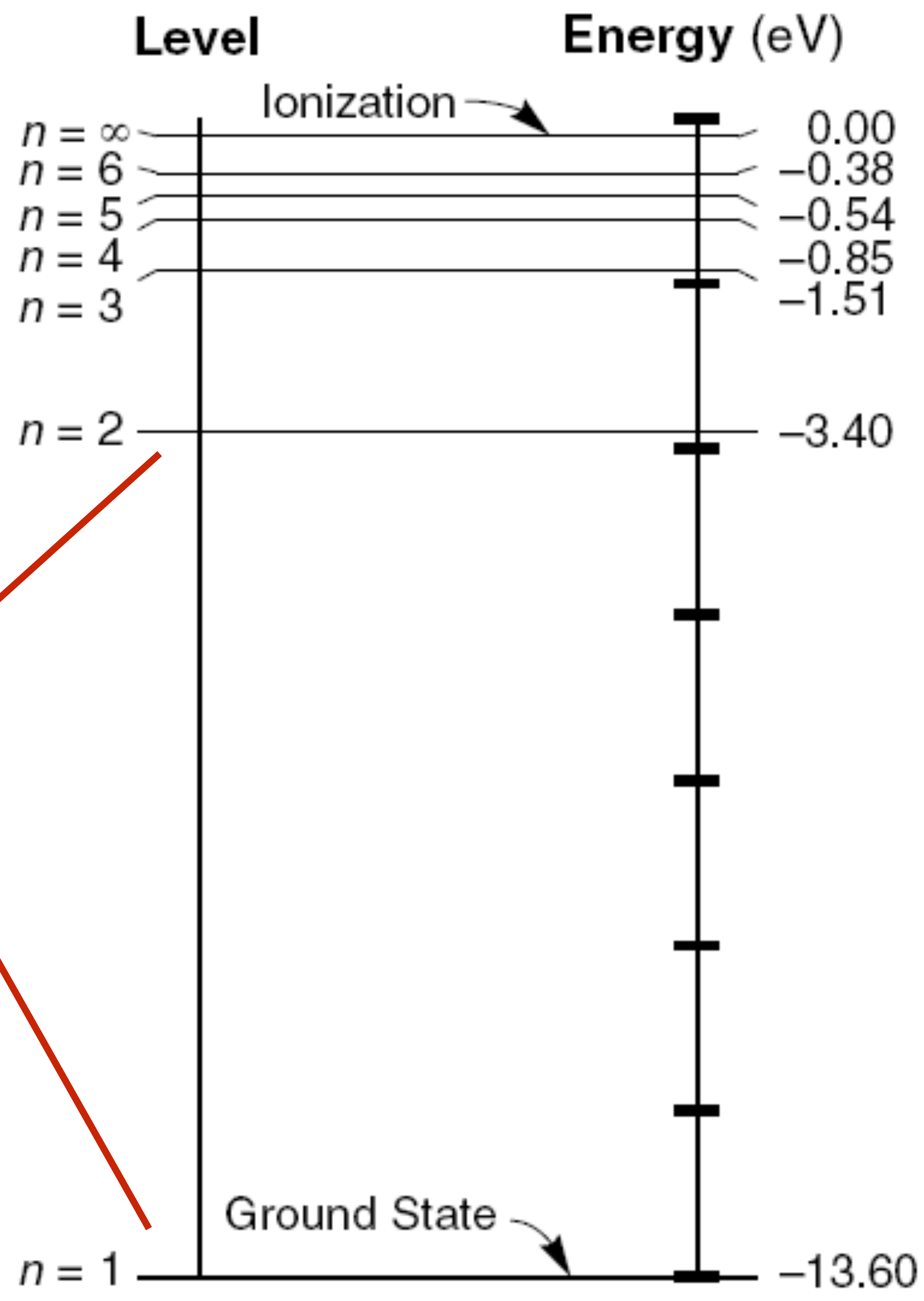
Step 1: relate the internal excitation states of each ionization states

Boltzmann factor

“Multiplicity” of an energy level
(How many electrons can fit?)

$$\frac{P(\text{State a})}{P(\text{State b})} = \frac{n_a}{n_b} = \frac{g_a}{g_b} e^{-(|E_a - E_b|)/kT}$$

Hydrogen $g(n) = 2n^2$



Energy Levels for the Hydrogen Atom

$$\frac{n_2}{n_1} = \frac{8}{2} e^{-(10.21\,\text{eV})/kT}$$

For a given ionization state (e.g. H^o):

An excited state "s"

$$\frac{n_s}{n_o} = \frac{g_s}{g_o} e^{-\epsilon_s/kT}$$

The ground state

An excited state "s"

As a function of the ground state

$$n_s = \frac{n_o}{g_o} \; g_s \; e^{-\epsilon_s/kT}$$

$$n = n_o + n_1 + n_2 + \ldots$$

$$n = \sum_s n_s = \frac{n_o}{g_o} \; g_0 \; e^{-\epsilon_o/kT} + \frac{n_o}{g_o} \; g_1 \; e^{-\epsilon_1/kT} + \frac{n_o}{g_o} \; g_2 \; e^{-\epsilon_2/kT} + \ldots$$

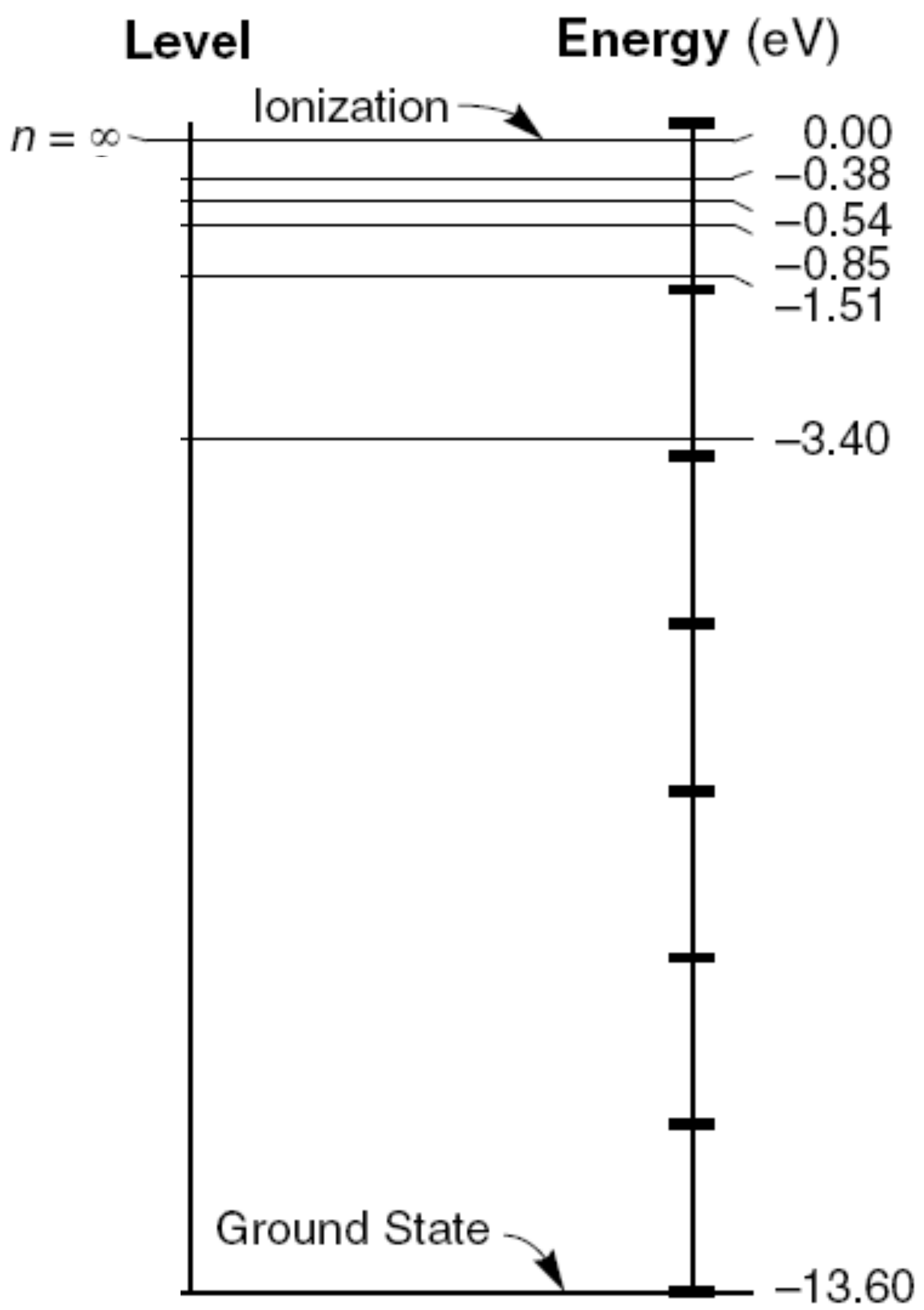
$$n = \frac{n_o}{g_o} \boxed{\sum_s \; g_s \; e^{-\epsilon_s/kT}}$$

$$n^r = \frac{n_o^r}{g_o^r} \boxed{U^r(T, s_{\max})}$$

"Partition function"

If we know the structure of the atom, we can calculate it

Hydrogen $g(n) = 2n^2$



Energy Levels for the Hydrogen Atom

There is a relation between the total population of a given ionization state (e.g H^o) and the population of that ion's ground state (e.g. H^o_o)

$$A^r_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^-$$

Goal: find $\dfrac{n^r_A}{n_A}$

1a $n^r = \dfrac{\boxed{n^r_o}}{g^r_o} U^r(T)$ (e.g. H^o):

1b $n^{r+1} = \dfrac{\boxed{n^{r+1}_o}}{g^{r+1}_o} U^{r+1}(T)$ (e.g. H^+):

. . .

(Until we reach the completely ionized state)

Unknowns:

n^r n^{r+1}

n^r_o n^{r+1}_o

Step 2: now the idea will be to relate the population of the ground stares of both ionization states together.

Let's consider the ionization reactions from ground state to ground state:

Goal: find $\dfrac{n_A^r}{n_A}$

$$A_o^r \; + \underbrace{\text{energy}}_{\chi_r^{r+1} + \boxed{\frac{p_e^2}{2m_e}}} \Longleftrightarrow A_o^{r+1} + e^-$$

$$\frac{P(\text{State a})}{P(\text{State b})} = \frac{n_a}{n_b} = \frac{g_a}{g_b} e^{-\left(\chi_r^{r+1} + \frac{p_e^2}{2m_e} \right)/kT}$$

Goal: find $\dfrac{n_A^r}{n_A}$

$$A_o^r \; + \text{energy} \Longleftrightarrow A_o^{r+1} + e^-$$

State b

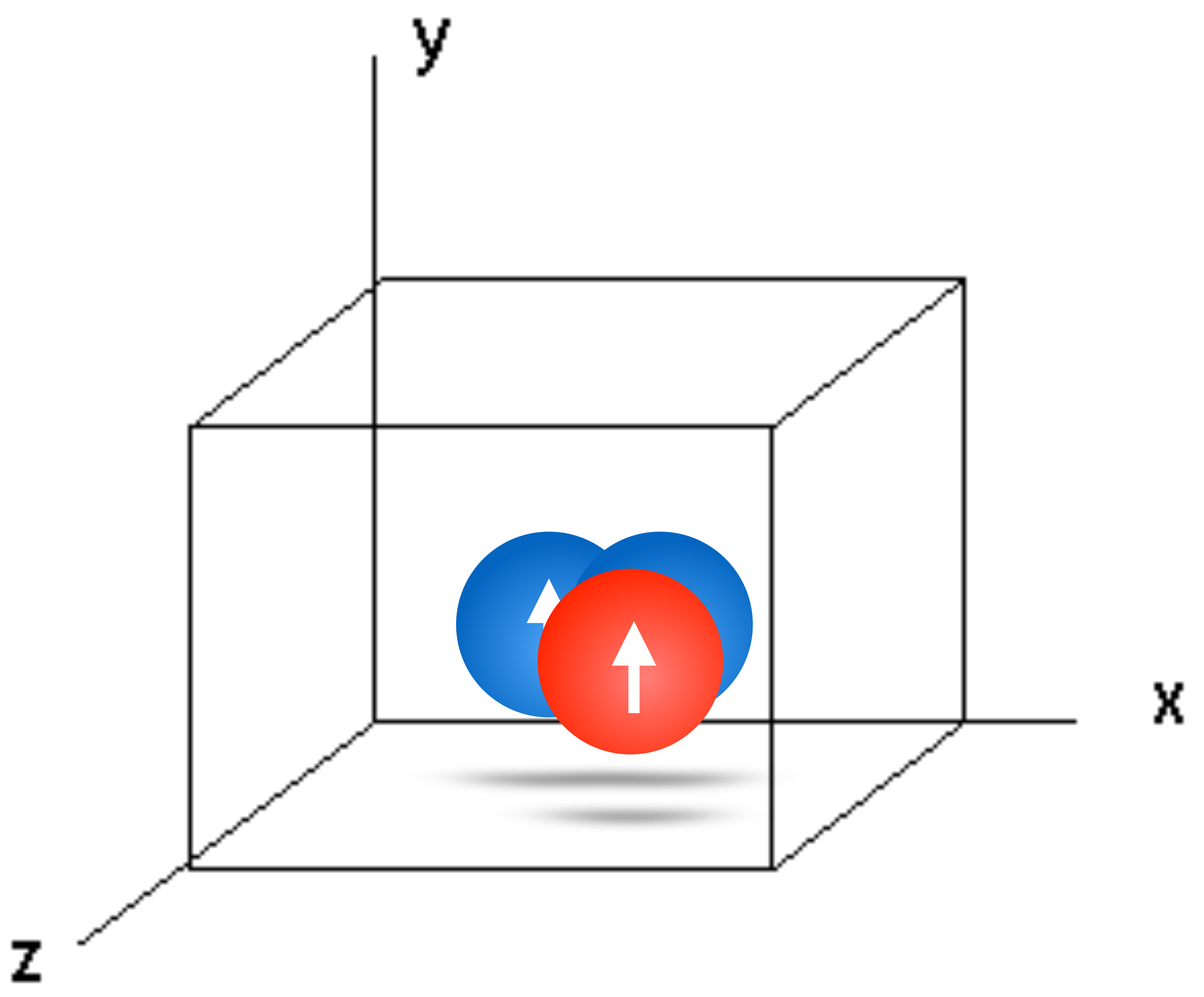
State a :includes the state of the free electron!

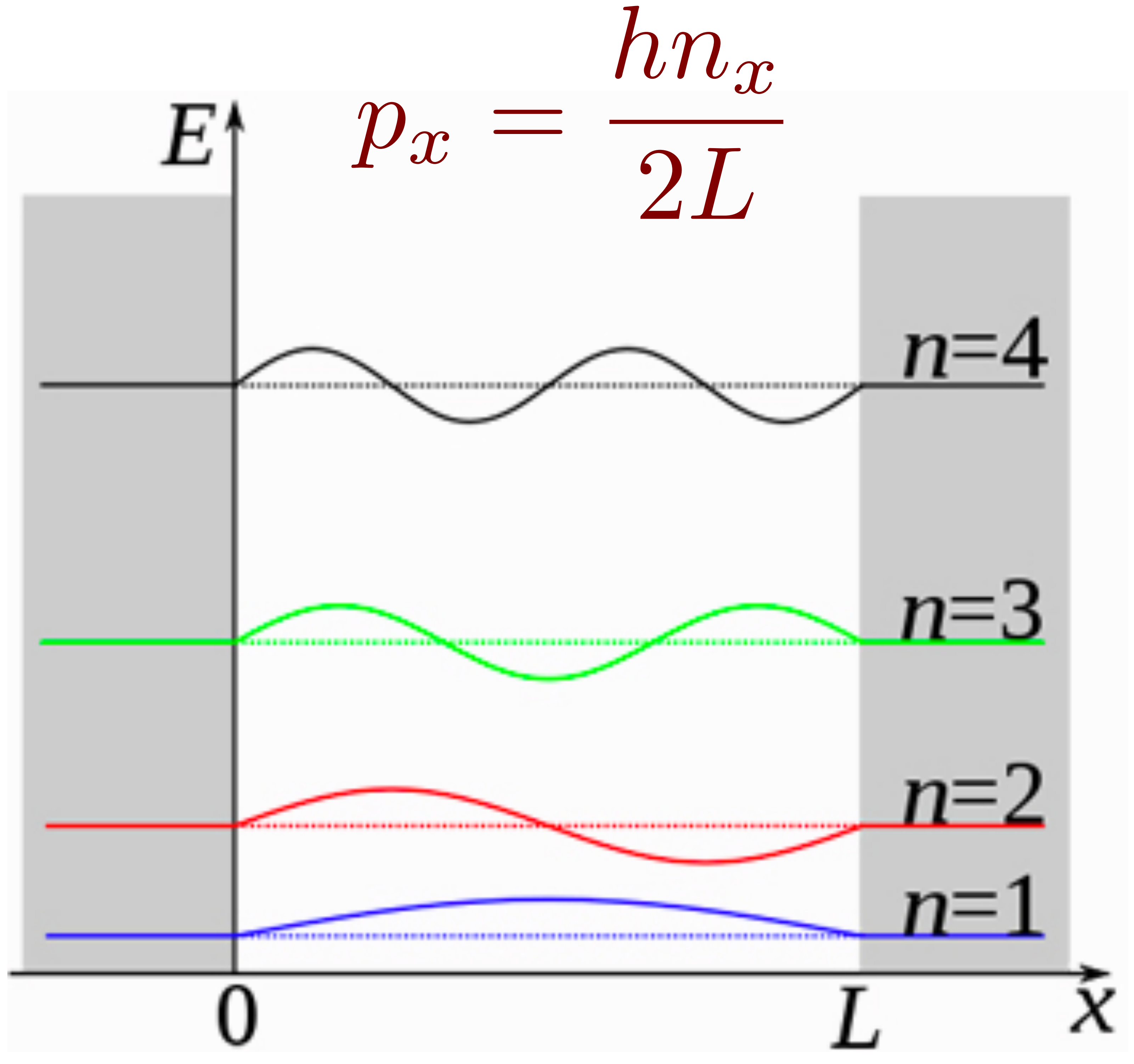
$g_b = g_o^r$

$g_a = g_o^{r+1} g_e$

What is the multiplicity of the electron?

$$\frac{P(\text{State a})}{P(\text{State b})} = \frac{n_a}{n_b} = \frac{g_a}{g_b} e^{-\left(\chi_r^{r+1} + \frac{p_e^2}{2m_e} \right)/kT}$$





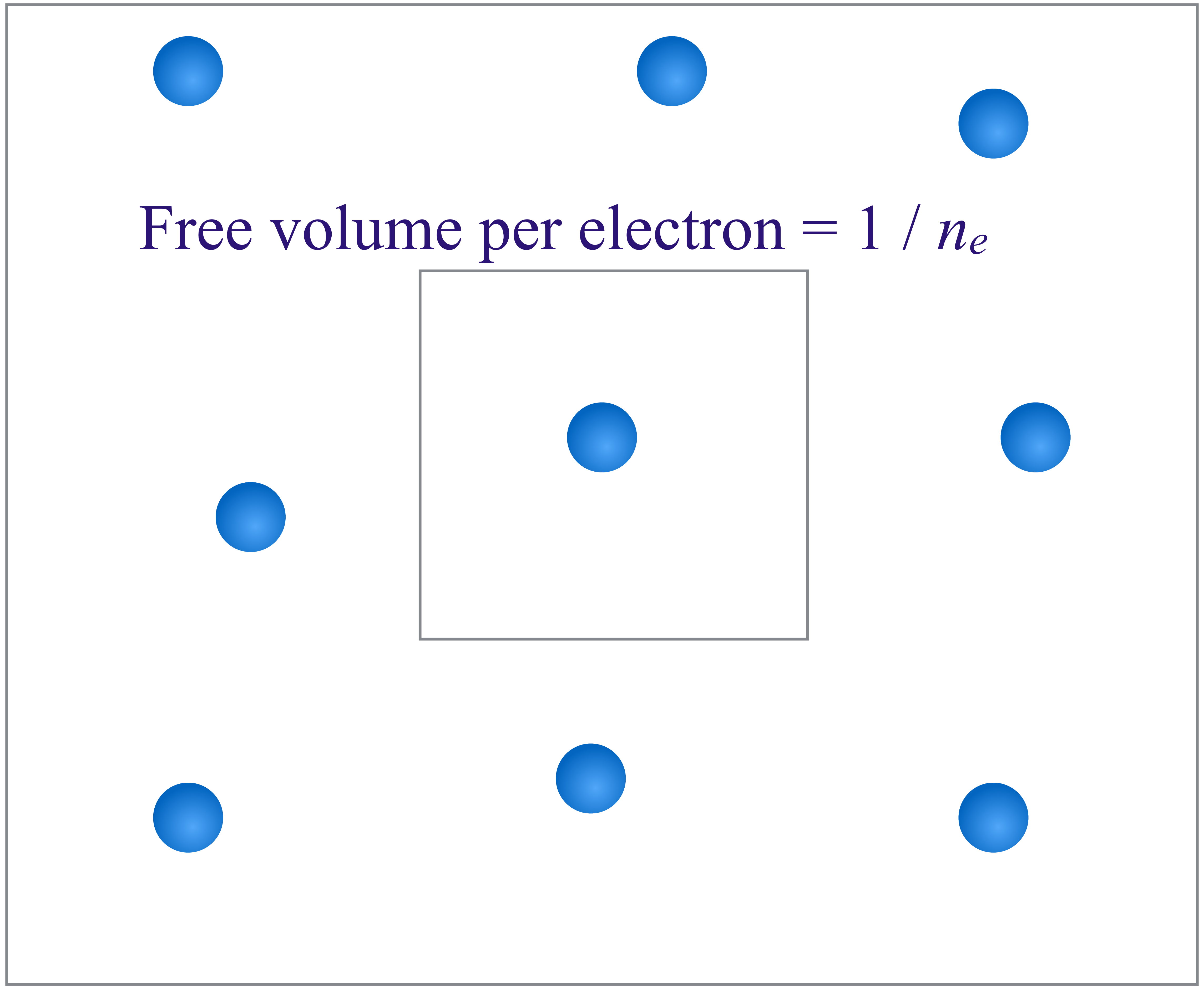
$$\Delta p_x \Delta x \sim h$$
$$\Delta p_y \Delta y \sim h$$
$$\Delta p_z \Delta z \sim h$$

Free electron “personal” space:

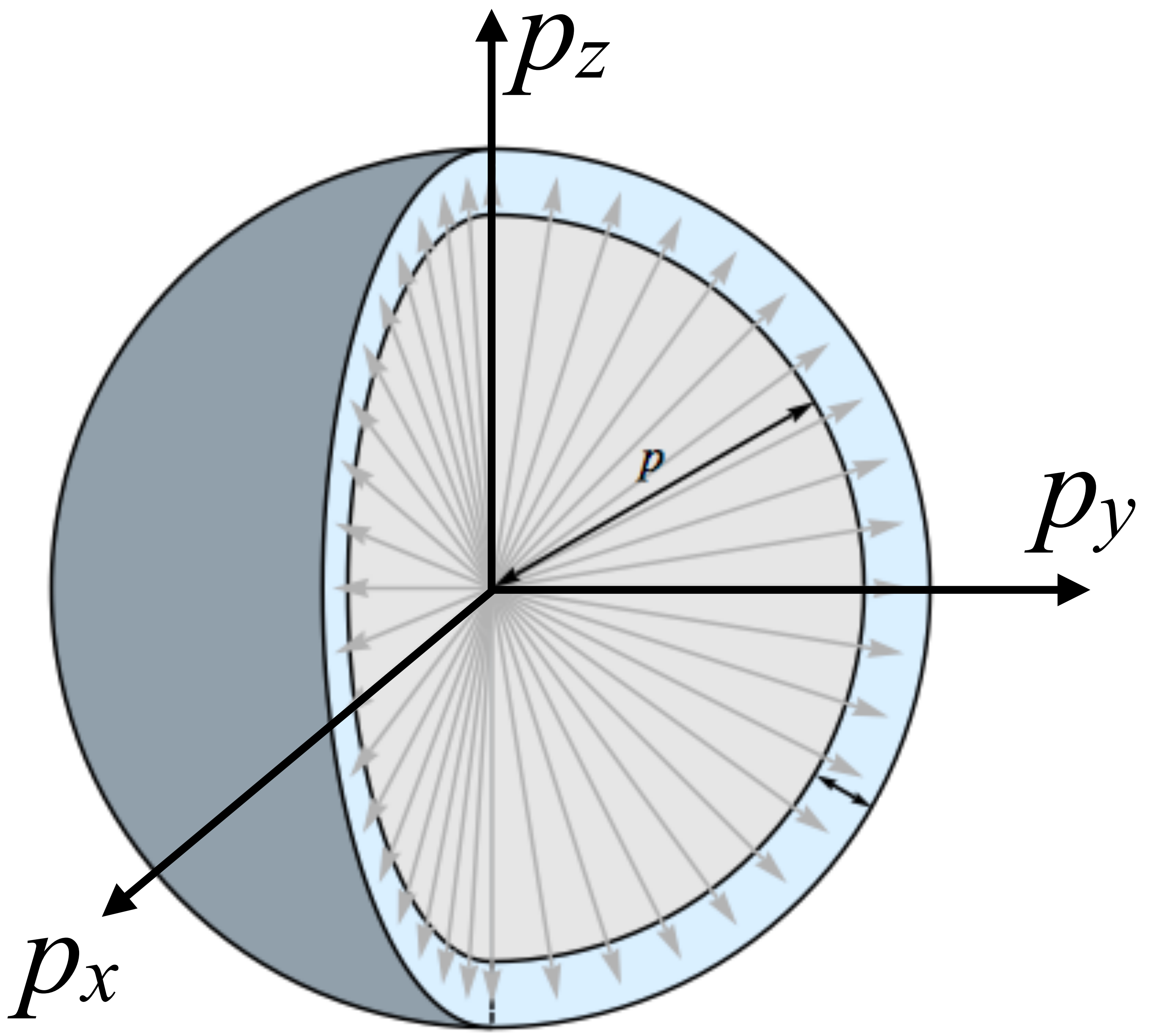
$$\delta V \delta p_x \delta p_y \delta p_z = h^3$$

Multiplicity of an electron with momentum between p and $p+dp$

$$d\,g_e = 2\,\frac{\text{Total volume * Total "momentum volume"}}{\text{Free electron "personal" space }(h^3)} = 2\frac{4\pi p^2\,dp}{n_e h^3}$$



"Momentum volume" for an electron with momentum between p and $p+dp = 4\pi p^2 dp$.



$$dg_e = \frac{8\pi}{n_e h^3} p_e^2 dp_e$$

$$\frac{n_b}{n_a} = \int_{p=0}^{\infty} \frac{g_o^{r+1} g_e}{g_o^r} e^{-(\chi_r^{r+1} + \frac{p_e^2}{2m_e})/kT}$$

Change of variable

$$x^2 = \frac{p_e^2}{2m_e kT}$$

$$\frac{n_b}{n_a} = \int_{p=0}^{\infty} \frac{g_o^{r+1}}{g_o^r} e^{-(\chi_r^{r+1} + \frac{p_e^2}{2m_e})/kT} \frac{8\pi}{n_e h^3} p_e^2 dp_e$$

$$\frac{n_b}{n_a} = \frac{g_o^{r+1}}{g_o^r} \frac{2(2\pi m_e kT)^{3/2}}{n_e h^3} e^{-\chi_r^{r+1}/kT}$$

$$\frac{n_b}{n_a} n_e = \frac{g_o^{r+1}}{g_o^r} \frac{2(2\pi m_e kT)^{3/2}}{h^3} e^{-\chi_r^{r+1}/kT}$$

$$A^r_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^-$$

Goal: find $\dfrac{n^r_A}{n_A}$

1a $$n^r = \frac{n^r_o}{g^r_o} U^r(T)$$

1b $$n^{r+1} = \frac{n^{r+1}_o}{g^{r+1}_o} U^{r+1}(T)$$

...

2a $$\frac{n^{r+1}_o}{n^r_o} n_e = \frac{g^{r+1}_o}{g^r_o} \frac{2(2\pi m_e kT)^{3/2}}{h^3} e^{-\chi_r/kT}$$

...

Unknowns:

n^r n^{r+1}

n^r_o n^{r+1}_o

n_e

$$P_e = n_e kT$$

In equation 3, substitute the ground state population for the total population with eps 1 and 2

$$\frac{n^{r+1}}{n^r} \boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

$$\frac{n^{r+1}}{n^r} \boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

Relate this "electron pressure" to the total gas pressure

$$P_{\text{total}} = n_{\text{free}} \; kT$$

$$= \frac{(n_{\text{ion}} + n_e)}{n_e} \; kT \, n_e$$

$$= \frac{(n_{\text{ions}} + n_e)}{n_e} \; P_e$$

$$P_e = \frac{n_e / n_{\text{ion}}}{\frac{n_{\text{ion}}}{n_{\text{ion}}} + \frac{n_e}{n_{\text{ion}}}} \; P_{\text{tot}}$$

$$P_e = \frac{E}{1 + E} \; P_{\text{tot}}$$

$$K_r^{r+1}(T, P)$$

$$\frac{n^{r+1}/n_{\text{ion}}}{n^r/n_{\text{ion}}} \frac{E}{1+E} = \boxed{\frac{T^{5/2}}{P_{\text{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}}$$

Saha for a known P and T

$$K_r^{r+1}(T,P) = \frac{T^{5/2}}{P_{\text{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

$$x^r = \frac{n^r_{\text{ion}}}{n_{\text{ion}}}$$

$U^r(T,P)$: Partition function

$$E = \frac{n_e}{n_{\text{ions}}}$$

Number of free electron per ion

For each element in the gas mixture:

1 $$\frac{x^{r+1}}{x^r} \frac{E}{1+E} = K_r^{r+1}(T,P)$$

$\cdots$

2 $$\sum_r x^r = 1$$

Unknowns:

x^r $\quad$ x^{r+1} $\quad$ $\cdots$

E

3 Charge conservation:
How does E relates to all the x^r (of all elements)?

Saha for a known P and T for pure Hydrogen

$$K_r^{r+1}(T,P) = \frac{T^{5/2}}{P_{\mathrm{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

For each element in the gas mixture:

1 $$\frac{x^{r+1}}{x^r}\frac{E}{1+E} = K_r^{r+1}(T,P) \quad \Rightarrow \quad \frac{x_{\mathrm{H}}^{+}}{x_{\mathrm{H}}^{o}}\frac{E}{1+E} = K_o^{+}(T,P)$$

...

2 $$\sum_r x^r = 1 \quad \Rightarrow \quad x_{\mathrm{H}}^{+} + x_{\mathrm{H}}^{o} = 1$$

3 Charge conservation:
How does E relates to all the x^r (of all elements)?

$$\Rightarrow \quad E = x_{\mathrm{H}}^{+}$$

$$E = \frac{n_e}{n_{\mathrm{ions}}}$$

Solve for *E*: $$E = \left(\frac{K_o^{+}}{K_o^{+}+1}\right)^{1/2}$$